

SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

Product Identifier

SRM Number: 1656

SRM Name: Thianthrene Combustion Calorimetric Standard

Other Means of Identification: Not applicable.

Recommended Use of This Material and Restrictions of Use

This Standard Reference Material (SRM) s intended for use in checking the suitability of apparatus, analytical procedures, and calculations involved in oxygen-bomb calorimetry of organic sulfur compounds. A unit of SRM 1656 consists of approximately 30 g of high purity thianthrene.

Company Information

National Institute of Standards and Technology Standard Reference Materials Program 100 Bureau Drive, Stop 2300 Gaithersburg, Maryland 20899-2300

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2. HAZARDS IDENTIFICATION

Classification

Physical Hazard: Not classified. **Health Hazard:** Not classified.

Label Elements

Symbol

No symbol/No pictogram.

Signal WordNo signal word.

Hazard Statement(s): Not applicable.

Precautionary Statement(s): Not applicable.

Hazards Not Otherwise Classified: Not applicable.

Ingredients(s) with Unknown Acute Toxicity: Not applicable.

3. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Substance: Thianthrene

Other Designations: Dibenzo-para-dithin; diphenylene disulfide; $C_{12}H_8S_2$. Components are listed in compliance with OSHA's 29 CFR 1910.1200.

Hazardous Component(s)	CAS Number	EC Number (EINECS)	Nominal Mass Concentration (%)
Thianthrene	92-85-3	202-197-0	100

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4. FIRST AID MEASURES

Description of First Aid Measures

Inhalation: If adverse effects occur, remove to well-ventilated (uncontaminated) area. If not breathing, qualified personnel should give artificial respiration. Seek immediate medical attention.

Skin Contact: Rinse affected skin with water for at least 15 minutes, then wash thoroughly with soap or mild detergent and water. If skin irritation persists, seek medical aid and bring the container or label.

Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes.

Ingestion: If a large amount is swallowed, get medical attention.

Most Important Symptoms/Effects, Acute and Delayed: May cause mild or mechanical eye, skin, or respiratory tract irritation.

Indication of any immediate medical attention and special treatment needed, if necessary: If any of the above symptoms are present, seek immediate medical attention.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards: Slight fire hazard. Dust/air mixtures may ignite or explode. See Section 9, "Physical and Chemical Properties" for flammability properties.

Extinguishing Media

Suitable: Regular dry chemical, carbon dioxide, water, or alcohol-resistant foam.

Unsuitable: None listed.

Specific Hazards Arising from the Chemical: Not applicable.

Special Protective Equipment and Precautions for Fire-Fighters: Move container from fire area if it can be done without personal risk. Avoid inhalation of material or combustion by-products. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus (SCBA).

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NFPA Ratings (0 = Minimal; 1 = Slight; 2 = Moderate; 3 = Serious; 4 = Severe)
Health = 1 Fire = 1 Reactivity = 0
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6. ACCIDENTAL RELEASE MEASURES

Personal Precautions, Protective Equipment and Emergency Procedures: Use suitable protective equipment; see Section 8, "Exposure Controls and Personal Protection". Keep out of waters supplies and sewers.

Methods and Materials for Containment and Clean up: Collect in appropriate container for disposal.

7. HANDLING AND STORAGE

Safe Handling Precautions: Avoid dust formation. Avoid breathing vapors, mist or gas. See Section 8, "Exposure Controls and Personal Protection".

Storage and Incompatible Materials: Store in a well-ventilated area. Keep separated from incompatible substances (see Section 10, "Stability and Reactivity").

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Exposure Limits: No occupational exposure limits have been established for thianthrene. This material is a crystalline material and adequate inhalation/respiratory protection should be used to minimize exposure.

Particulates Not Otherwise Regulated (PNOR)

OSHA (PEL): 15 mg/m³ (TWA, total dust)

5 mg/m³ (TWA, respirable fraction)

NIOSH (REL): 15 mg/m³ (TWA, total dust)

5 mg/m³ (TWA, respirable fraction)

Engineering Controls: Provide local exhaust or process enclosure ventilation system. Ensure compliance with applicable exposure limits.

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Personal Protection Measures: In accordance with OSHA 29 CFR 1910.132, subpart I, wear appropriate Personal Protective Equipment (PPE) to minimize exposure to this material.

Respiratory Protection: If workplace conditions warrant a respirator, a respiratory protection program that meets OSHA 29CFR 1910.134 must be followed. Refer to NIOSH 42 CFR 84 for applicable certified respirators.

Eye Protection: Splash resistant safety goggles and emergency eyewash are recommended.

Skin and Body Protection: Chemical resistant clothing and gloves are recommended.

9. PHYSICAL AND CHEMICAL PROPERTIES

Properties	Thianthrene	
Molar Mass (g/mol)	216.30	
Molecular Formula	$C_{12}H_8S_2$	
Appearance (physical state, color, etc.)	solid crystals	
Odor	not available	
Odor threshold	not available	
pН	not available	
Evaporation rate	not available	
Melting point/freezing point	153 °C to 159 °C (307 °F to 318 °F)	
Relative Density (water = 1)	not available	
Density	not available	
Vapor Pressure	not available	
Vapor Density (air = 1)	not available	
Viscosity	not available	
Solubilities	water: insoluble	
Partition coefficient (n-octanol/water)	not available	
Thermal Stability Properties		
Autoignition Temperature	· · · · · · · · · · · · · · · · · · ·	
Thermal Decomposition	364 °C to 366 °C (687 °F to 690 °F)	
Initial boiling point and boiling range	not available	
Explosive Limits, LEL (Volume %)	not available	
Explosive Limits, UEL (Volume %)	not available	
Flash Point (Closed Cup)	not available	
Flammability (solid, gas)	not available	

10. STABILITY AND REACTIVITY

Reactivity: Stable at normal temperatures and pressure.							
							Stability: X Stable
Possible Hazardous Reactions: Not applicable.							
Conditions to Avoid: Avoid heat, flames, sparks and other sources of ignition.							
Incompatible Materials: Oxidi:	zing materials.						
Hazardous Decomposition: Oxides of sulfur and carbon.							
Hazardous Polymerization	Will Occur	X	Will Not Occur				

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11. TOXICOLOGICAL INFORMATION Inhalation X Skin **Route of Exposure:** X X Ingestion Symptoms Related to the Physical, Chemical and Toxicological Characteristics: Irritation of skin, eye or respiratory tract may occur. Potential Health Effects (Acute, Chronic, and Delayed) **Inhalation:** May cause irritation. **Skin Contact:** May cause irritation with redness and burning. Eye Contact: Contact may cause irritation with redness. **Ingestion:** May cause irritation. **Numerical Measures of Toxicity Acute Toxicity:** Not classified; no data available. Skin Corrosion/Irritation: Not classified. Serious Eye Damage/Eye Irritation: Not classified; no data available. Respiratory Sensitization: Not classified; no data available. **Skin Sensitization:** Not classified; no data available. Germ Cell Mutagenicity: Not classified; no data available. Carcinogenicity: Not classified. Listed as a Carcinogen/Potential Carcinogen Yes Thianthrene is not listed by IARC, NTP or OSHA as a carcinogen or potential carcinogen. **Reproductive Toxicity:** Not classified; no data available. STOT, Single Exposure: Not classified; no data available. STOT, Repeated Exposure: Not classified; no data available. **Aspiration Hazard:** Not applicable. 12. ECOLOGICAL INFORMATION **Ecotoxicity Data:** No data available. Persistence and Degradability: No data available. **Bioaccumulative Potential:** No data available. Mobility in Soil: No data available. Other Adverse effects: No data available. 13. DISPOSAL CONSIDERATIONS **Waste Disposal:** Dispose in accordance with all applicable federal, state, and local regulations. 14. Transportation Information **U.S. DOT and IATA:** This material is not regulated by DOT or IATA. 15. REGULATORY INFORMATION **U.S. Regulations** CERCLA Sections 102a/103 (40 CFR 302.4): Not regulated. SARA Title III Section 302 (40 CFR 355.30): Not regulated. SARA Title III Section 304 (40 CFR 355.40): Not regulated.

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SARA Title III Section 313 (40 CFR 372.65): Not regulated. OSHA Process Safety (29 CFR 1910.119): Not regulated.

SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21):

ACUTE HEALTH: No CHRONIC HEALTH: No FIRE: No REACTIVE: No PRESSURE: No

State Regulations

California Proposition 65: Not regulated.

U.S. TSCA Inventory: Thianthrene is listed.

TSCA 12(b), Export Notification: Not listed.

Canadian Regulations: WHMIS Information is not provided for this material.

16. OTHER INFORMATION

Issue Date: 27 May 2015

Sources: ChemADVISOR, Inc., SDS *Thianthrene*, 20 March 2015.

CDC; NIOSH; NIOSH Pocket Guide to Chemical Hazards; Department of Health and Human Services (DHHS), Centers for Disease Control and Prevention (CDC), National Institute for Safety and Health; Particulates Not Otherwise Regulated, 4 April 2011; available at

http://www.cdc.gov/niosh/npg/npgd0480.html (accessed May 2015)

Key of Acronyms:

ACGIH	American Conference of Governmental Industrial Hygienists	NTP	National Toxicology Program
CAS	Chemical Abstracts Service	OSHA	Occupational Safety and Health Administration
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act	PEL	Permissible Exposure Limit
CFR	Code of Federal Regulations	RCRA	Resource Conservation and Recovery Act
DOT	Department of Transportation	REL	Recommended Exposure Limit
EINECS	European Inventory of Existing Commercial Chemical	RQ	Reportable Quantity
	Substances		
EPCRA	Emergency Planning and Community Right-to-Know Act	RTECS	Registry of Toxic Effects of Chemical Substances
IARC	International Agency for Research on Cancer	SARA	Superfund Amendments and Reauthorization Act
IATA	International Air Transportation Agency	SCBA	Self-Contained Breathing Apparatus
IDLH	Immediately Dangerous to Life and Health	SRM	Standard Reference Material
LC50	Lethal Concentration	STOT	Specific Target Organ Toxicity
LD50	Median Lethal Dose or Lethal Dose, 50 %	STEL	Short Term Exposure Limit
LEL	Lower Explosive Limit	TLV	Threshold Limit Value
MSDS	Material Safety Data Sheet	TPQ	Threshold Planning Quantity
NFPA	National Fire Protection Association	TSCA	Toxic Substances Control Act
NIOSH	National Institute for Occupational Safety and Health	TWA	Time Weighted Average
NIST	National Institute of Standards and Technology	UEL	Upper Explosive Limit
n.o.s.	Not Otherwise Specified	WHMIS	Workplace Hazardous Materials Information System

Disclaimer: Physical and chemical data contained in this SDS are provided only for use in assessing the hazardous nature of the material. The SDS was prepared carefully, using current references; however, NIST does not certify the data in the SDS. The values for this material are given in the NIST Certificate of Analysis.

Users of this SRM should ensure that the SDS in their possession is current. This can be accomplished by contacting the SRM Program: telephone (301) 975-2200; fax (301) 948-3730; e-mail srmmsds@nist.gov; or via the Internet at http://www.nist.gov/srm.

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